

$P4_122$

D_4^3

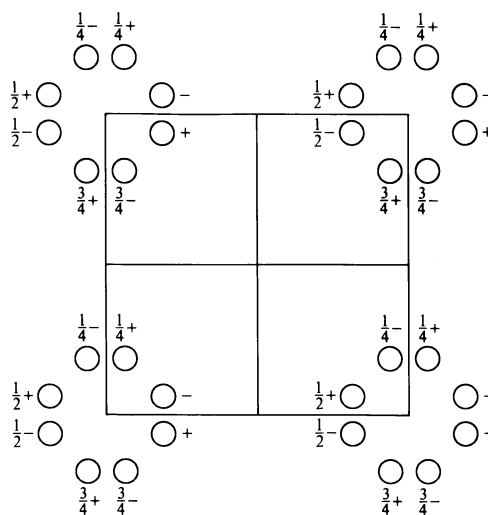
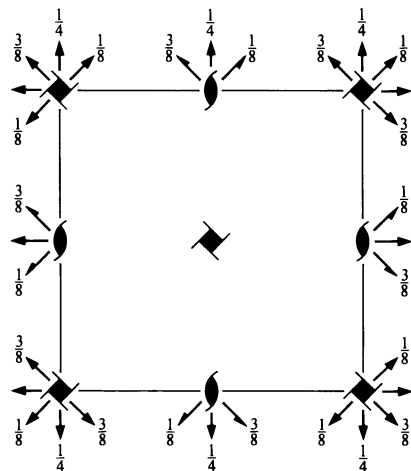
422

Tetragonal

No. 91

$P4_122$

Patterson symmetry $P4/mmm$



Origin on $2[010]$ at $4_1(1,2)1$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{8}$

Symmetry operations

- (1) 1
- (2) $2(0,0,\frac{1}{2})$ $0,0,z$
- (3) $4^+(0,0,\frac{1}{4})$ $0,0,z$
- (4) $4^-(0,0,\frac{3}{4})$ $0,0,z$
- (5) 2 $0,y,0$
- (6) 2 $x,0,\frac{1}{4}$
- (7) 2 $x,x,\frac{3}{8}$
- (8) 2 $x,\bar{x},\frac{1}{8}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
8 <i>d</i> 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{1}{4}$	(4) $y,\bar{x},z+\frac{3}{4}$	General: $00l: l = 4n$
	(5) \bar{x},y,\bar{z}	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{3}{4}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{4}$	Special: as above, plus $0kl: l = 2n + 1$ or $l = 4n$
4 <i>c</i> ..2	$x,x,\frac{3}{8}$	$\bar{x},\bar{x},\frac{7}{8}$	$\bar{x},x,\frac{5}{8}$	$x,\bar{x},\frac{1}{8}$	$hhl: l = 2n + 1$ or $l = 4n$
4 <i>b</i> .2.	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},\frac{1}{2}$	$\bar{y},\frac{1}{2},\frac{1}{4}$	$y,\frac{1}{2},\frac{3}{4}$	$hhl: l = 2n + 1$ or $l = 4n$
4 <i>a</i> .2.	$0,y,0$	$0,\bar{y},\frac{1}{2}$	$\bar{y},0,\frac{1}{4}$	$y,0,\frac{3}{4}$	$hhl: l = 2n + 1$ or $l = 4n$

Symmetry of special projections

Along $[001]$ $p4mm$
 $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
 Origin at $0,0,z$

Along $[100]$ $p2gm$
 $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,0,\frac{1}{4}$

Along $[110]$ $p2gm$
 $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
 Origin at $x,x,\frac{3}{8}$